

2,3,4-Trinitrotoluene
602-29-9 | DTXSID60208944

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.90e-05 mmHg

Global applicability domain: Outside

Local applicability domain index: 3.33e-01

Confidence level: 5.07e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Methylbutanoic acid</div> <div>Measured: 8.02e-06</div> <div>Predicted: 4.22e-01</div>	<div>Image not found</div> <div>Dicloran</div> <div>Measured: 6.44e-06</div> <div>Predicted: 4.17e-06</div>	<div>Image not found</div> <div>3,4,5-Trimethylphenyl methylcarbamate</div> <div>Measured: 6.00e-04</div> <div>Predicted: 9.97e-05</div>
<div>Image not found</div> <div>2-(Diisopropylamino)ethanol</div> <div>Measured: 8.49e-05</div> <div>Predicted: 2.32e-01</div>	<div>Image not found</div> <div>Benzoyl chloride</div> <div>Measured: 9.00e-04</div> <div>Predicted: 3.80e-01</div>	